Materials Matter

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Measurements in high magnetic fields aid understanding of twodimensional materials

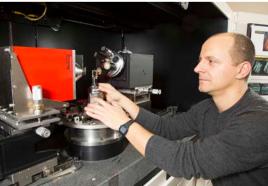
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Celebrating service

Heads UP!







Clockwise from left: Inside the Los Alamos National Laboratory fuel cell test lab, graduate students and a postdoctoral researcher work on ElectroCat technology-from back, Joseph **Dumont, Ulises Martinez,** and Ling Lin; Dusan Spernjak (previously an MPA-11 postdoctoral researcher with the fuel cell program. now an R&D engineer, AET-1) performs x-ray computed microtomography to nondestructively 3D image fuel cell components; postdoctoral researcher Xi Yin (MPA-11) synthesizes a PGM-free catalyst.

Los Alamos and Argonne team up to develop more affordable fuel cell components

Researchers at DOE's Los Alamos and Argonne national laboratories have teamed up to support a DOE initiative through the creation of the Electrocatalysis Consortium (ElectroCat), a collaboration devoted to finding an effective but cheaper alternative to platinum and platinum group metals in hydrogen fuel cells.

ElectroCat is dedicated to finding new ways to replace rare and costly platinum group metals in fuel cell cathodes with more accessible and inexpensive substitutes, such as materials based on the earth-abundant metals iron and cobalt.

Piotr Zelenay (Materials Synthesis and Integrated Devices, MPA-11) is lead scientist on the Los Alamos component of the consortium.

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Learning about the exciting science that is going on in our division firsthand from you makes the highlight of my day.



From Tanja's desk ...

Here it is April, which means that I have been with LANL for two months! Thank you all for the warm welcome. My very special thanks go out to Susie, Rick, and the rest of the MPA Leadership Team who tirelessly answer my many questions and help me get acquainted with our division and LANL in general.

My primary goal for my first year is to get to know you, and I have met most of you at least in passing over the course of four group meetings. I have begun to get together with you in smaller teams. Learning about the exciting science that is going on in our division firsthand from you makes the highlight of my day.

Rick and I are in full gear preparing for this year's Materials Capability Review that will focus on the Materials Strategy refresh, dynamic materials, and MaRIE. Leadership of this activity is swapped between MST and MPA, and this year it is MPA's turn. Fortunately, we have many helpers. Several of you have been tapped for posters and presentations, and your attention to all requests in a timely manner will help us run a successful review resulting in constructive feedback. However, consider this activity not merely an event for our external review committee. This also is a great opportunity to showcase our capabilities to the rest of the Lab, and hopefully serve as a platform to spur new joint activities. Since one of our topics at the capability review is the strategy refresh, there obviously is activity on this topic! Our Materials Strategy is captured in the *Vistas* document, published last in 2010 and thus worthy of a fresh look. Consider this document as the North Star of all materials activities—materials research at LANL is so broad and diverse that it is worthwhile to spell out our common goals in a guiding document.

I can't pass up on the opportunity to ask for your help—in my eight years at NSF and DOE/BES I learned how important it is for us to share the exciting science that is happening every day. Your time helping to produce highlights, working with Karen and her team and the program managers at the agencies to make them digestible so that a reasonably educated public can see the impact, is well spent. We have a lot of competition and we have to convince our sponsors that they made the right decision. Also, never forget that our federal support ultimately is provided by the taxpayer, so we owe it to them to make our research accessible.

Lastly, I want to reiterate an offer that I extended at the group meetings—if there is anything that you want to run by me, my door is open. You can usually catch me in the office before 9 a.m.; after that, my day tends to fill up with meetings and you may want to check with Susie first on my availability.

I am very excited to be here and look forward to working with you.

MPA Division Leader Tanja Pietraß



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I appreciate now that a "what-if" analysis and properly addressing the potential hazards of my "hobby" could have saved me from a nearly fatal accident.



From Chuck's desk

The sixth arrow

A great deal of the work that we do at LANL is highly complex with the potential for very serious consequences. The very nature of research is that the outcome is unknown—things can go wrong and they do. What is essential and sets us apart is how we learn and share these experiences. Overcoming my own sense of self-consciousness, I share one of the most harrowing moments of my life. I appreciate now that a "what-if" analysis and properly addressing the potential hazards of my "hobby" could have saved me from a near-fatal accident.

When I was about 19 years old and out hunting, I installed a tree stand, attached a homemade fall restraint, and sat down. I hoisted up my bow and arrows and sat quietly—perched in a tree (about eight meters above the ground); five arrows in the quiver and one on the string, all with razor-blade tips (known as broadheads). After sitting in the tree stand for about 2.5 hours, the subtle sound of leaves crunching under hoof broke the silence. I slowly and methodically shifted my weight forward with hope to catch a glimpse of an approaching white-tailed deer. In a fraction of a second I felt myself dropping straight down as if a trap door on a hangman's gallows had released below me. It happened so quickly and unexpectedly that the only thought I can remember having at about half the way down was "arrows!" When I hit the ground, my head struck a fallen limb about five centimeters in diameter and I lost consciousness. I was deep in the forest, miles from the nearest paved road, cell phones did not yet exist, I was alone—no means of communication, fully camouflaged (hunter orange is not required for bow hunting), and in one of about five potential locations that only one or two friends could possibly find.

That is a string of bad decisions that I realized I had made and owned the consequences of. Suddenly I saw daylight and my immediate thought was again "arrows!" I was lying on five arrows with razor broadheads still in the protective guiver. Where was the sixth? Horrified of the potential situation, I jumped up and ran my hands across my midsection and chest hoping not to find the sixth arrow impaled in my body. I did not find it! Thank goodness! This was happening very quickly, seemingly in about a second or two. On my first breath there was a problem. Very little air was going in. I coughed into my hand and blood spattered into my palm. I sensed pain at multiple places on my arms, legs, torso, neck, and head. I again ran my hands across my midsection, chest, and back hoping to NOT find the missing arrow. Fortunately, it eluded me. I struggled to get enough air to satisfy my lungs. Again I coughed, and more blood. I knew something was gravely wrong and that I had to get out of there and get medical attention. My truck was parked about one kilometer from my tree stand. A few steps into my walk out, I realized that I had broken my nose fairly high up and it was bleeding internally. It hurt, but a forceful pinch to the bridge of my nose stopped the blood flow: I could feel it abate immediately. The pain was severe, but I made it out of the woods.

The point in sharing this real-life story is that we each own our safety. Clearly I made some very bad decisions, and for the tiniest of perturbations, the arrow that somehow landed about two meters away could have been driven through me and I never would have made it more than a few steps. My bad decisions nearly cost me my life. Learning from that string of bad decisions starts by reflecting and sharing so that we can improve everyone's safety. Learning and sharing is key to Step Five of ISM and it is how we make progress towards being better tomorrow than we are today.

NHMFL Pulsed Field Facility Director and Condensed Matter and Magnet Science Deputy Group Leader Chuck Mielke

MPA staff in the news

Andrew Baker honored with poster and student awards for fuel cell durability research

Graduate research assistant Andrew Baker (Materials Synthesis and Integrated Devices, MPA-11) won Best Poster Award and a second place Bernard Baker Student Award at the 2015 Fuel Cell Seminar and Energy Exposition, held in Los Angeles. The meeting is the premier United States



conference for the fuel cell and hydrogen industry.

A PhD candidate in mechanical engineering from the University of Delaware, Baker joined the Laboratory in 2014 to continue his dissertation studies on polymer electrolyte membrane (PEM) fuel cell durability. His award-winning poster, "Cerium migration during PEM fuel cell operation," investigates the effect of cerium moving between layers of the membrane electrode assembly (MEA) at the core of fuel cells. Cerium is used to enhance the durability of fuel cells by diffusing chemical attacks. However, migration of cerium ions within the cells during operation may decrease local performance and durability. Baker's elemental mapping techniques explore mechanisms that influence cerium movement in operating fuel cells. Understanding such factors will enable the development of cerium additives with increased stability, which could extend the durability of PEM fuel cells. Dennis Torraco, Rangachary Mukundan, and Rod Borup (MPA-11); Dusan Spernjak (Applied Engineering Technology, AET-1); Beth Judge (Chemical Diagnostics and Engineering, C-CDE); and University of Delaware collaborators participated in the research, which the DOE Fuel Cell Technologies Office funded.

Baker also received the second place Bernard Baker Student Award for his experimental studies of PEM fuel cell durability. His research addresses the mechanical and chemical durability of PEM fuel cells through the development of novel composite membranes, as well as understanding the migration of cerium during cell operation. The award is named in honor of Bernard Baker (no relation), who devoted his career to fuel cells used for generating electric power. The award gives financial support to exceptional students in the field of fuel-cell-related technologies. The Bernard S. Baker Fuel Cell Scholarship Fund provides a cash prize, and the Fuel Cell Seminar & Energy Exposition provides supplemental funds and free registration for the 2015 Fuel Cell Seminar & Energy Exposition.

Technical contact: Andrew Baker

Marc Janoschek selected for Hans Fischer Fellowship

Marc Janoschek (Condensed Matter & Magnet Science, MPA-CMMS), has been selected for a Hans Fischer Fellowship at the Technical University of Munich (TUM) Institute for Advanced Study in Germany. Under the three-year fellowship named for TUM professor Hans Fischer, who was



awarded the 1930 Nobel Prize in Chemistry, Janoschek will perform research aimed at improving the understanding of complex material properties that emerge in quantum matter at the extremes of high pressure.

The fellowship enables exceptional early-career international scientists to explore cutting-edge, high-risk topics in their scientific research areas in partnership with a TUM research group.

At the Munich research reactor, Janoschek and TUM collaborator Christian Pfleiderer will use novel state-of-the-art neutron-resonance spin-echo (NRSE) spectroscopy techniques that provide unprecedented energy resolution in order to investigate the emergent properties of quantum matter. Janoschek's fellowship research, outlined in his proposal "New Frontiers of Neutron Spectroscopy in Quantum Matter," aligns with the research he carries out within the program "Complex Electron Materials" that is funded by the Department of Energy's Office of Basic Energy Sciences (DOE-OBES), as well as with the grand challenges outlined by DOE and the Lab's Materials for the Future science pillar.

Janoschek performed his doctoral studies in solid-state physics at the Paul Scherrer Institut in Switzerland and at TUM, where he graduated summa cum laude. He was a Feodor-Lynen postdoctoral fellow of the German Alexander von Humboldt Foundation at the University of California, San Diego, in the group of Brian Maple. Since 2011, Janoschek has been the capability leader for neutron scattering in MPA-CMMS.

Technical contact: Marc Janoschek

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MPA staff cont.

Jarek Majewski named 2016 NSSA Fellow

Jaroslaw (Jarek) Majewski (Center for Integrated Nanotechnologies, MPA-CINT) is a 2016 Neutron Scattering Society of America (NSSA) Fellow. The society recognized Majewski "for contributions to our understanding of weakly organized two-dimensional systems, including surfactant molecules found in biological systems."



Majewski, who performs his research at the Lujan Neutron Scattering Center and CINT, received his PhD in materials and interfaces from the Weizmann Institute of Science. Israel. He performed research in HASYLAB, Germany; the Advanced Photon Source, Argonne National Laboratory; Risø National Laboratory, Denmark; the National Institute of Standards and Technology; and Oak Ridge National Laboratory. He joined Los Alamos as a Director's Funded Postdoctoral Fellow and became a staff member in 1997. In 2005. Majewski was named an American Physical Society Fellow for his contributions to understanding the structural properties of Langmuir films and model biomembranes at solidliquid interfaces using x-ray and neutron scattering. He is an adjunct professor at the Department of Chemical Engineering at the University of California, Davis and the recipient of several Los Alamos awards, including a 2007 Los Alamos National Laboratory Director Distinguished Performance Award.

Through the NSSA Fellowship Program, NSSA recognizes members who have made significant contributions to the neutron scattering community in North America through original research and publication, innovative applications of neutron scattering, contributions to the promotion or development of neutron scattering, or participation in the activities of the NSSA or neutron community.

The Neutron Scattering Society of America was formed in 1992 and organizes members from more than 26 countries with interest in neutron scattering research in a wide spectrum of disciplines. No more than one-half of one percent of members are honored as fellows through election by the Fellowship Committee.

Technical contact: Jarek Majewski

IEEE Van Duzer Prize for best manuscript goes to Doan Nguyen and co-authors

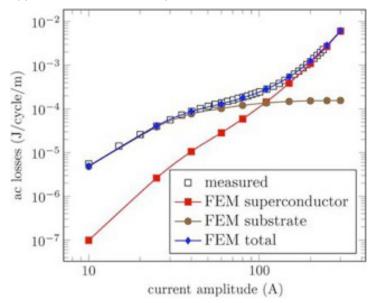
Doan Nguyen (Materials Physics Applications, Condensed Matter & Magnet Science) and his co-authors will receive the 2014 IEEE Van Duzer Prize for their manuscript "Computation of losses in HTS under the action of varying magnetic fields and currents," which appeared as an invited review paper



in IEEE Transactions on Applied Superconductivity. The award will be given at the 2016 Applied Superconductivity Conference, to be held in September in Denver.

Sponsored by the IEEE Council on Superconductivity, the Van Duzer Prize recognizes the best contributed paper published in IEEE Transactions on Applied Superconductivity during each volume year. Papers are evaluated on the expectation that the paper will be highly cited by future authors, technical excellence of the work described, and completeness of the paper as an archival record of a finished body of research.

Alternatiing current (AC) losses are arguably one of the most challenging problems remaining for superconducting applications and accurate prediction of AC loss in



FEM and experimental results for the AC loss components in a 1-cm-wide RABiTS YBCO tape with ferromagnetic NiW substrate (Ic = 330 A) carrying an AC transport current. The FEM model developed at LANL is capable of taking the non-linear interaction between ferromagnetic substrate and HTS layer to reproduce well the measured data.

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high-temperature superconducting (HTS) wires/devices is important to optimize the design of HTS systems. Los Alamos provided a review on its advanced finite element model to accurately calculate AC loss and electromagnetic dynamics in a combined system of superconductors and ferromagnetic materials.

The majority of the research was done in support of DOE's HTS power applications projects funded through the Laboratory's former Superconductivity Technology Center. A small fraction of the work to refine the model was funded by the Laboratory Directed Research and Development program. The work supports the Laboratory's Energy Security mission and Materials for the Future science pillar.

Reference: "Computation of Losses in HTS Under the Action of Varying Magnetic Fields and Currents," by Francesco Grilli (Karlsruhe Institute of Technology, Germany), Enric Pardo (Slovak Academy of Sciences, Bratislava, Slovakia), Antti Stenvall (Tampere University of Technology Tampere, Finland), Doan N. Nguyen (MPA-CMMS), Weijia Yuan (University of Bath, Bath), and Fedor Gömöry (Slovak Academy of Sciences, Bratislava, Slovakia) IEEE Transactions on Applied Superconductivity, 24, 1, (2014).

Technical contact; Doan Nguyen

Filip Ronning recognized as distinguished mentor

Filip Ronning (Condensed Matter and Magnet Science, MPA-CMMS) is a recipient of a Laboratory Postdoctoral Distinguished Mentor Award. The awards recognize the positive and significant impact a Los Alamos National Laboratory mentor has had on a postdoctoral researcher's experience at the Lab by providing outstanding leadership, guidance, and career advice substantially beyond what would normally be expected.



Filip Ronning was nominated for his unwavering dedication to the academic and personal well-being of his postdocs. He is an extremely successful and knowledgeable scientist and leads projects that consistently allow postdocs to produce high-quality publications. Ronning is generous with his knowledge and expertise-making himself available to discuss scientific ideas and helping postdocs with writing presentations or papers. His kind and open manner encourages the free discussion of ideas, enabling the postdocs' growth in understanding and confidence. Ronning's genuine interest in the career development of his postdocs

goes well beyond what might normally be expected. He encourages the postdocs to pursue their own interests and develop skills that will help them in their future careers. Ronning provides career guidance, planning, and networking. Moreover, he helps new postdocs settle into life in Los Alamos, particularly helping foreign nationals find their footing in a new country. All the postdocs who have had the pleasure of working with Ronning are delighted to see him rewarded for the outstanding contribution he has made to their time at Los Alamos. Nicholas Wakeham (MPA-CMMS) nominated Ronning.

Technical contact: Filip Ronning

Sandberg elected to leadership of LCLS Users' Executive Committee

Richard Sandberg has been elected vice-chair of the Linac Coherent Light Source (LCLS) Users' Executive Committee. A committee member since 2014, he will lead the committee in helping to improve user operations and facility capabilities. He will become committee chair in October.



Opened in 2009 at the Department of Energy's SLAC National Accelerator Laboratory in California. LCLS is the world's

first hard x-ray laser. It has enabled Sandberg and collaborators to create the first-ever in situ images of void collapse in explosives using an x-ray free electron laser (XFEL).

Sandberg (Center for Integrated Nanotechnologies, MPA-CINT) holds a PhD in physics, with a certificate in optics, from the University of Colorado Boulder. He joined LANL in 2009 as a Director's Postdoctoral Fellow and became a staff scientist in 2011.

LCLS includes six experimental stations and attracts proposals in a range of disciplines that include biology; soft and hard materials; matter in extreme conditions; chemistry; atomic, molecular and optical; and methods and instrumentations. Sandberg's discipline is matter in extreme conditions. Use of LCLS is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

Key technologies originally developed at Los Alamos in the 1980s and 1990s, such as the radio frequency photoinjector and high-brightness electron beams, enabled the XFEL facilities currently in use worldwide. Moreover, Los Alamos was part of a multi-laboratory collaboration that designed

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MPA staff cont.

and built the Linac Coherent Light Source.

Los Alamos's proposed experimental facility MaRIE (Matter-Radiation Interactions in Extremes) will be the world's highest energy hard XFEL. Used for time-dependent materials research, it will help researchers like Sandberg design the advanced materials needed to meet 21st-century national security and energy security challenges.

Technical contact: Richard Sandberg

Measurements in high magnetic fields aid understanding of two-dimensional materials

In 2010, a new family of atomically thin semiconductors was discovered: the monolayer transition metal dichalcogenides (TMDs), which include materials such as molybdenum disulfide (MoS₂) and tungsten diselenide (WSe₂). These materials have a similar two-dimensional honeycomb structure to graphene but with an important and technologically relevant difference. Unlike graphene, monolayer TMDs possess a sizable semiconductor bandgap, which makes them potentially useful for future applications in electronics and electrooptics. The study of these new TMD semiconductors is an active area of research in materials science and condensed matter physics. Los Alamos researchers and collaborators have performed optical studies of TMDs in high pulsed magnetic fields. *Nature Communications* published their research findings.

The elementary excitation in any semiconductor is the exciton, an electron in the conduction band that is electrostatically bound to a hole in the valence band. Excitons are created by absorption of light, and their radiative recombination gives rise to optical emission (luminescence). The fundamental properties of excitons in many new TMD semiconductors—i.e., their size, mass, binding energy, and magnetic moment—are largely unknown and have not been directly observed experimentally.

Researchers at the National High Magnetic Field Laboratory (NHMFL) in Los Alamos used large area monolayer TMD films, grown by collaborators at the U.S. Naval Research Laboratory, for optical reflection spectroscopy studies of atomically thin tungsten disulfide (WS₂) and MoS₂ crystals in very high pulsed magnetic fields to 65 T. These measurements revealed the magnetic moment of the fundamental excitons and also, for the first time, their physical size. The parameters can be used to constrain estimates of the exciton binding energy itself, which is crucial for future applications in lasing and solar energy harvesting.

Historically, magneto-optical measurements have played an essential role in determining the fundamental parameters of electronic excitations in bulk and quantum-confined

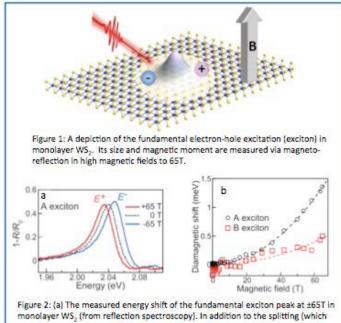


Figure 2: (a) The measured energy shift of the fundamental exciton peak at ±65T in monolayer WS₂ (from reflection spectroscopy). In addition to the splitting (which reveals magnetic moment), the average peak position reveals (b), the quadratic diamagnetic exciton shift, from which the exciton radius is directly inferred (1.53 nm for the "A" exciton).

semiconductors. In conventional semiconductors, such as gallium arsenide, electron/hole masses and exciton binding energies are small; consequently, magnetic fields only of order 10 T are sufficient to reveal the small quadratic spectral shift of the exciton's optical transition (the exciton diamagnetic shift), from which the exciton size and binding energy can be directly inferred.

However, excitons in the new family of monolayer TMD semiconductors are very strongly bound (and consequently they are very small), such that very large magnetic fields exceeding approximately 40 T are necessary to reveal these fundamental parameters. The new paper reported observation of the quadratic shift of both the "A" and "B" exciton in monolayer WS $_{\rm 2}$ at low temperatures and in 65 T magnetic fields.

Reference: "Exciton Diamagnetic Shifts and Valley Zeeman Effects in Monolayer WS₂ and MoS₂ to 65 T," Nature Communications **7**, 10643 (2016). Authors: Andreas V. Stier and Scott A. Crooker (Condensed Matter and Magnet Science, MPA-CMMS), Kathleen M. McCreary and Berend T. Jonker (Naval Research Laboratory), Junichiro Kono (Rice University).

The team performed the optical studies at the National High Magnetic Field Laboratory, which the National Science Foundation and the State of Florida fund. The research supports the Lab's Energy Security mission area and Materials for the Future science pillar by revealing the physical parameters for this new family of atomically thin semiconductors. *Technical contact: Scott Crooker*

Affordable fuel cell components cont.

ElectroCat is one of four consortia that makes up DOE's Energy Materials Network (EMN). The EMN will facilitate industry access to the unique scientific and technical resources available at the national laboratories, enabling manufacturers to bring advanced materials to market more quickly.

The partnership between Argonne and Los Alamos that forms the core of ElectroCat involves the study, creation, and implementation of possible alternatives to platinum-based electrodes through material-development efforts headed by Los Alamos and accelerated by the high-throughput, combinatorial, characterization, and electrode performance modeling capabilities at Argonne, as well as by applying a high-performance supercomputer to model new catalyst structures at Los Alamos.

In developing new materials to be explored, researchers at Los Alamos will bring to bear 15 years of experience in non-precious metal catalyst design, synthesis, characterization, and testing. In addition, Los Alamos can apply multiscale modeling techniques that leverage world-class computing facilities to design catalysts with optimal activity, selectivity, and durability. The work supports the Laboratory's Energy Security mission and Materials for the Future science pillar.

Once the potential replacement candidate materials are identified, scientists in the consortium will examine materials using a number of different methods, including x-ray imaging and spectroscopy techniques at Argonne. Argonne researchers can also investigate samples in a number of different environments that replicate how they would function in real-world scenarios.

By combining the expertise and capabilities at Los Alamos and Argonne, in partnership with the private sector and universities, researchers expect to accelerate the development and implementation of platinum group metal-free catalysts in fuel cells.

Technical contact: Piotr Zelenay

Celebrating service

Congratulations to the following MPA Division employee recently celebrating a service anniversary:

Anatoly Efimov, MPA-CINT......15 years

HeadsUP!

Safety leadership: Reinvigorating HPI

Applying the understanding of human behaviors and the role they play in work processes to improve performance in safety and productivity is the essence of human performance improvement (HPI). In a new Safety Leadership campaign column, int.lanl.gov/safety/safety-leadership/new-hpi-team.shtml, read how the Environment, Safety and Health Directorate recently brought in three individuals with HPI skills in targeted areas that complement the unique institutional needs of the Lab.

Safety alert: Use caution when driving through VAPs

Laboratory employees are reminded to be cognizant and alert for Centerra-Los Alamos protective force members when driving through vehicle access portals (VAPs). There have been a couple of near misses recently that involved protective force officers and vehicles driving through the VAPs.

Protective force officers have been asked to make eye contact with employees when returning employee badges and to wear safety vests when outside VAP booths. Employees are asked to proceed slowly through the VAP and look in both directions for protective force officers or other personnel who may be standing outside and/or near VAP booths.

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Materials Physics and Applications

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To submit news items or for more information, contact Karen Kippen, ADEPS Communications, at 505-606-1822 or kkippen@lanl.gov. To read past issues see www.lanl.gov/orgs/mpa/materialsmatter.shtml.



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